Prediction of Microbial Growth Rate versus Biomass Yield by a Metabolic Network with Kinetic Parameters

Adadi, Roi; Volkmer, Benjamin; Milo, Ron; Heinemann, Matthias; Shlomi, Tomer

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TEXT S1

FVA formulation for MOMENT

The vector of enzyme concentrations, *g*, is unique due to the fact that each reaction is associated with a unique gene to reaction mapping, having different turnover number and molecular weight. We confirm this by applying a variant of Flux Variability
Analysis (FVA) on MOMENT's enzyme concentration vector, as following:

$$\max / \min \; g_i$$

$$\text{subject to} \; Sv = 0,$$

$$v_{lb} \le v \le v_{ub},$$

$$v_j \le kcat_j \cdot g_i \; \ldots \; \leftarrow \text{genes-to-reactions constraints,}$$

$$\sum g_i \cdot MW_i \le C \left[\frac{g_{protein}}{g_{DW}} \right],$$

$$c^T v = Z$$

Where Z is the optimal solution to the MOMENT problem:

$$\max \; c^T v$$

$$\text{subject to} \; Sv = 0,$$

$$v_{lb} \le v \le v_{ub},$$

$$v_j \le kcat_j \cdot g_i \; \ldots \; \leftarrow \text{genes-to-reactions constraints,}$$

$$\sum g_i \cdot MW_i \le C \left[\frac{g_{protein}}{g_{DW}} \right]$$

And c represents the biomass production's objective function.

The growth rate scales linearly with the threshold on the total enzyme mass

Changing the total enzyme mass in the model scales the growth rate linearly and therefore does not change the Pearson correlation between the measured and the predicted growth rate. If we denote by f the flux distribution obtained by MOMENT when using a threshold C on the total enzyme mass, then αf would be an optimal MOMENT solution when using a threshold of αC. Notably, this results from the fact that v_{lb} and v_{ub} are either –inf, 0, or +inf for all reactions v in the model – as we assume that specific data on nutrient uptake and secretion rates is unavailable.